

On the combinatorial structure of 0/1-matrices representing nonobtuse simplices

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Abstract

A 0/1-*simplex* is the convex hull of $n + 1$ affinely independent vertices of the unit n -cube I^n . It is *nonobtuse* if none its dihedral angles is obtuse, and *acute* if additionally none of them is right. Acute 0/1-simplices in I^n can be represented by 0/1-matrices P of size $n \times n$ whose Gramians $G = P^\top P$ have an inverse that is *strictly* diagonally dominant, with *negative* off-diagonal entries.

In this paper, we will prove that the positive part D of the transposed inverse $P^{-\top}$ of P is *doubly stochastic* and has the same support as P . In fact, P has a *fully indecomposable* doubly stochastic pattern. The negative part C of $P^{-\top}$ is strictly row-substochastic and its support is complementary to that of D , showing that $P^{-\top} = D - C$ has no zero entries and has positive row sums. As a consequence, for each facet F of an acute 0/1-facet S there exists *at most one* other acute 0/1-simplex \hat{S} in I^n having F as a facet. We call \hat{S} the *acute neighbor* of S at F .

If P represents a 0/1-simplex that is merely nonobtuse, the inverse of $G = P^\top P$ is only *weakly* diagonally dominant and has *nonpositive* off-diagonal entries. Consequently, $P^{-\top}$ can have entries equal to zero. We show that its positive part D is still doubly stochastic, but its support may be *strictly contained* in the support of P . This allows P to have no doubly stochastic pattern and to be *partly decomposable*. In theory, this might cause a nonobtuse 0/1-simplex S to have several *nonobtuse* neighbors \hat{S} at each of its facets.

In the remainder of the paper, we study nonobtuse 0/1-simplices S having a partly decomposable matrix representation P . We prove that if S has such a matrix representation, it also has a *block diagonal* matrix representation with at least two diagonal blocks. Moreover, *all* matrix representations of S will then be partly decomposable. This proves that the *combinatorial* property of having a fully indecomposable matrix representation with doubly stochastic pattern is a *geometrical* property of a subclass of nonobtuse 0/1-simplices, invariant under all n -cube symmetries. We will show that a nonobtuse simplex with partly decomposable matrix representation can be split in mutually orthogonal simplicial facets whose dimensions add up to n , and in which each facet has a fully indecomposable matrix representation. Using this insight, we are able to extend the *one neighbor theorem* for acute simplices to a larger class of nonobtuse simplices.

Keywords: Acute simplex; nonobtuse simplex; orthogonal simplex; 0/1-matrix; doubly stochastic matrix; fully indecomposable matrix; partly decomposable matrix.

1 Introduction

A 0/1-simplex is an n -dimensional 0/1-polytope [18] with $n + 1$ vertices. Equivalently, it is the convex hull of $n + 1$ of the 2^n elements of the set \mathbb{B}^n of vertices of the unit n -cube

I^n whenever this hull has dimension n . Throughout this paper, we will study 0/1-simplices modulo the action of the hyperoctahedral group \mathcal{B}_n of symmetries of I^n . As a consequence, we may assume without loss of generality that a 0/1-simplex S has the origin as a vertex. This makes it possible to represent S by a non-singular $n \times n$ matrix P whose columns are the remaining n vertices of S . Of course, this representation is far from unique, as is illustrated by the 0/1-tetrahedron in Figure 1. First of all, there is a choice which vertex of S is located at the origin. Secondly, column permutations of P correspond to relabeling of the nonzero vertices of S , and thirdly, row permutations correspond to relabeling of the coordinate axis.

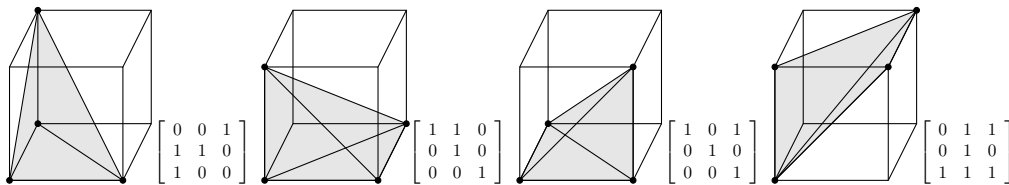


Figure 1: Matrix representations of the same 0/1-tetrahedron modulo the action of \mathcal{B}_3 .

We will be studying 0/1-simplices with certain geometric properties. These will be invariant under congruence, and in particular invariant under the action of \mathcal{B}_n , which forms a subset of the congruences of I^n . Thus, each of the matrix representations carries the required geometric information of the 0/1-simplex it represents. To be more specific, we will study the set of *acute* 0/1-simplices, whose dihedral angles are all acute, the *nonobtuse* 0/1-simplices, none of whose dihedral angles is obtuse, and the set of *orthogonal* simplices. An orthogonal simplex is a nonobtuse simplex with exactly n acute dihedral angles and $\frac{1}{2}n(n-1)$ right dihedral angles.

It is not difficult to establish that a 0/1-simplex S is nonobtuse if and only if the inverse $(P^\top P)^{-1}$ of the Gramian of any matrix representation P of S is a diagonally dominant Stieltjes matrix. This Gramian is *strictly* diagonally dominant and has even negative off-diagonal entries if and only if S is acute. See [4, 5, 7] for details. In this paper we will study the properties of the 0/1-matrices that represent acute, nonobtuse, and orthogonal simplices.

1.1 Motivation

The motivation to study nonobtuse simplices goes back to their appearance in finite element methods [3, 10] to approximate solutions of PDEs, in which triangulations consisting of nonobtuse simplices can be used to guarantee discrete maximum and comparison principles [8]. We then found that they figure in other applications, see [9] and the references therein. In the context of 0/1-simplices and 0/1-matrices, it is well known [14] that the *Hadamard conjecture* [15] is equivalent to the existence of a *regular* 0/1-simplex in each n cube with $n-3$ divisible by 4. Note that a regular simplex is always acute. Thus, studying acute 0/1-simplices can be seen as an attempt to study the Hadamard conjecture in new context, which is wider, but not too wide. Indeed, acute 0/1-simplices, although present in any dimension, are still very rare in comparison to *all* 0/1-simplices. See [5], in which we describe the computational generation of acute 0/1-simplices, as well as several mathematical properties. This paper can be seen as a continuation of [5], in which some new results on acute 0/1-simplices are presented, as well as on the again slightly larger class of nonobtuse 0/1-simplices.

1.2 Outline

We start in Section 2 with some preliminaries related to the hyperoctahedral group of cube symmetries, to combinatorics, and to the linear algebra behind the geometry of nonobtuse and acute simplices. We refer to [5] for much more detailed information on the hyperoctahedral group and combinatorial aspects, and to [9] for applications of nonobtuse simplices. In Section 3 we present our new results concerning *sign properties* of the *transposed inverses* $P^{-\top}$ of matrix representations P of acute 0/1-simplices S . These results imply that the matrices P are *fully indecomposable* with *doubly stochastic pattern* [11]. From this follows the so-called *one neighbor theorem*, which states that all $(n-1)$ -facets F of S are *interior* to the cube, and that each is shared by at most one other acute 0/1-simplex in I^n . See [6] for an alternative proof of that fact. If S is merely a nonobtuse 0/1-simplex, the support of P only *contains* a doubly stochastic pattern, and moreover, P can be *partly decomposable*. In Section 4 we study the matrix representations of such nonobtuse 0/1-simplices with partly decomposable matrix representations. The main conclusion is that each of them consists of p with $2 \leq p \leq n$ mutually orthogonal facets F_1, \dots, F_p of respective dimensions k_1, \dots, k_p that add up to n . Moreover, each $k_j \times k_j$ matrix representation of each facet F_j is fully indecomposable. In case all facets F_1, \dots, F_n are one-dimensional, the corresponding 0/1-simplex is a so-called *orthogonal simplex*, as it has a spanning tree of mutually orthogonal edges. Orthogonal 0/1-simplices played an important role in the nonobtuse cube triangulation problem, solved in [6]. We briefly recall them in Section 5 and put them into the novel context of Section 4. Finally, in Section 6 we use the insights developed so far to prove a one neighbor theorem for a wider class of nonobtuse simplices.

2 Preliminaries

Let $\mathbb{B} = \{0, 1\}$, and write $\mathbb{B}^n = \mathbb{B}^{n \times 1}$ for the set of vertices of the unit n -cube $I^n = [0, 1]^n$, which also contains the standard basis vectors e_1^n, \dots, e_n^n and their sum e^n , the *all-ones vector*. The 0/1-matrices of size $n \times k$ we denote by $\mathbb{B}^{n \times k}$. For each $X \in \mathbb{B}^{n \times k}$, define its *antipode* \overline{X} by

$$\overline{X} = e^n(e^k)^\top - X, \quad (1)$$

and write

$$\mathbf{1}(X) = (e^n)^\top X e^k \quad \text{and} \quad \mathbf{0}(X) = \mathbf{1}(\overline{X}) \quad (2)$$

for the number of entries of X equal to one, and equal to zero, respectively. For any $n \times k$ matrix X define its *support* $\text{supp}(X)$ by

$$\text{supp}(X) = \{(i, j) \in \{1, \dots, n\} \times \{1, \dots, k\} \mid (e_i^n)^\top X e_j^k \neq 0\}. \quad (3)$$

We now recall some concepts from combinatorial matrix theory [11, 12].

Definition 2.1 A nonnegative matrix A has a *doubly stochastic pattern* if there exists a doubly stochastic matrix $D = (d_{ij})$ such that $\text{supp}(D) = \text{supp}(A)$.

Definition 2.2 A matrix $A \in \mathbb{B}^{n \times n}$ is *partly decomposable* if there exists a $k \in \{1, \dots, n-1\}$ and permutation matrices Π_1, Π_2 such that

$$\Pi_1^\top A \Pi_2 = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}, \quad (4)$$

where A_{11} is a $k \times k$ matrix and A_{22} an $(n - k) \times (n - k)$ matrix. If Π_1 and Π_2 can be taken equal in (4) then A is called *reducible*. If A is not partly decomposable it is called *fully indecomposable*. If A is not reducible it is called *irreducible*.

Note that $A \in \mathbb{B}^{n \times n}$ is partly decomposable if and only if there exist nonzero $v, w \in \mathbb{B}^n$ with $\mathbf{1}(v) + \mathbf{1}(w) = n$ such that $v^\top A w = 0$, and that A is reducible if additionally, $w = \bar{v}$.

Lemma 2.3 *Let $X \in \mathbb{B}^{n \times n}$ be nonsingular and $X = [X_1 \mid X_2]$ a block partition of X where $X_1 \in \mathbb{B}^{n \times k}$ and $X_2 \in \mathbb{B}^{n \times (n-k)}$ for some $1 \leq k < n$. Suppose that $X_1^\top X_2 = 0$, and hence,*

$$X^\top X = \begin{bmatrix} X_1^\top X_1 & 0 \\ 0 & X_2^\top X_2 \end{bmatrix}. \quad (5)$$

Then there exists a permutation Π such that

$$\Pi X = \begin{bmatrix} X_{11} & 0 \\ 0 & X_{22} \end{bmatrix},$$

where $X_{11} \in \mathbb{B}^{k \times k}$ and $X_{22} \in \mathbb{B}^{(n-k) \times (n-k)}$ are nonsingular.

Proof. If $X_1^\top X_2 = 0$ then in particular $(e^k)^\top X_1^\top X_2 e^{n-k} = 0$, hence

$$\text{supp}(X_1 e^k) \cap \text{supp}(X_2 e^{n-k}) = \emptyset. \quad (6)$$

Since the rank of X_1 equals k , the support of $X_1 e^k$ consists of at least k indices. Similarly, the support of $X_2 e^{n-k}$ consists of at least $n - k$ indices. Thus, they consist of exactly k and $n - k$ indices. Now, let Π be a permutation that maps the support of $X_1 e^k$ onto $\{1, \dots, k\}$, then ΠX has the required form. \square

2.1 Matrix representations of 0/1-simplices modulo 0/1-equivalence

The convex hull of any subset $\mathcal{P} \subset \mathbb{B}^n$ is called a *0/1-polytope*. As a first simple and intuitive result, we explicitly show that no two distinct subsets of \mathbb{B}^n define the same 0/1-polytope.

Lemma 2.4 *Suppose that $V \in \mathbb{B}^{n \times k}$ has distinct columns and that $v \in \mathbb{B}^n$ is not a column of V . Then v is not a convex combination of the columns of V .*

Proof. Suppose that v is not a column of V and that $Vw = v$ for some $w \geq 0$. It suffices to show that $w^\top e^k \neq 1$. If $v = 0$ then V has no zero column, hence $w = 0$ is the only nonnegative vector solving $Vw = v$. If v has an entry equal to one, say $(e_\ell^n)^\top v = 1$, then $(e_\ell^n)^\top Vw = 1$, hence a non-empty subset $\mathcal{I} \subset \{1, \dots, k\}$ of the entries of w sums to one. In order to obtain $w^\top e^k = 1$, it is necessary that $\text{supp}(w) = \mathcal{I}$. Since $Vw \in \mathbb{B}^n$, this implies that each row of V has either only ones, or only zeros, at its entries at positions in \mathcal{I} . If \mathcal{I} has more than one element, then V has two or more columns that are equal, contradicting its definition. \square

This lemma proves the bijective correspondence between the power set of the 2^n vertices of I^n and the 0/1-polytopes. Since the cardinality $2^{(2^n)}$ of this power set is doubly exponential, the following concept makes sense. Two 0/1-polytopes will be called *0/1-equivalent* if they can be transformed into one another by the action of an element of the *hyperoctahedral group* \mathcal{B}_n of affine isometries $\mathbb{B}^n \rightarrow \mathbb{B}^n$. The group \mathcal{B}_n has $n!2^n$ elements and is generated by:

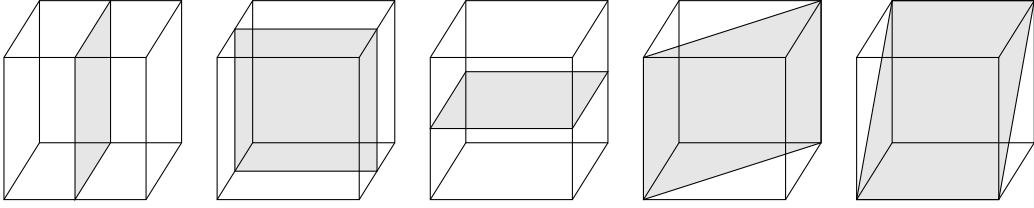


Figure 2: The five reflection planes corresponding to the octahedral group \mathcal{B}_3 .

- the n reflections in the hyperplanes $2x_i = 1$ for $i \in \{1, \dots, n\}$, and
- the $n - 1$ reflections in the hyperplanes $x_i = x_{i+1}$ for $i \in \{1, \dots, n - 1\}$.

See Figure 2 for the five reflection planes of \mathcal{B}_3 in I^3 .

Note that a reflection of the second type exchanges the values of the i th and $(i + 1)$ st coordinate. Hence, products of this type can result in any permutation of the coordinates.

A 0/1-*simplex* is a 0/1-polytope in I^n with $n + 1$ affinely independent vertices. We will study the set \mathbb{S}^n of 0/1- simplices in I^n modulo the action of \mathcal{B}_n . Therefore we can without loss of generality assume that one of its vertices is located at the origin, after which S can be conveniently represented by any square matrix whose columns are its remaining n vertices. Modulo the action of \mathcal{B}_n , two matrices describe the same 0/1-simplex if and only if one can

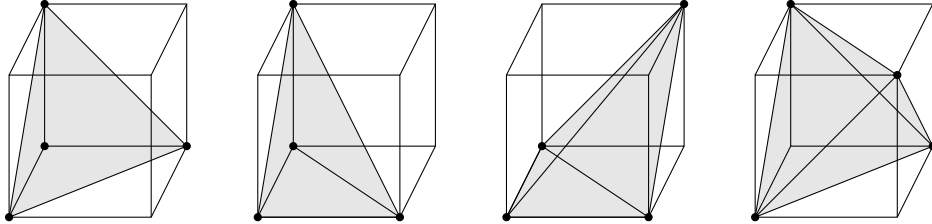


Figure 3: The only four 0/1-tetrahedra in I^3 modulo the action of \mathcal{B}_3 . In dimension 5 and higher there exist congruent simplices that are not equal modulo \mathcal{B}_n .

be obtained from the other using any combination of the following three operations,

(C) Column permutations;

(R) Row permutations;

(X) Select a column c and replace each remaining column d by $(c + d)(\text{mod } 2)$.

Operation (C) does not correspond to any action of \mathcal{B}_n , it just relabels the vertices of S . Operations of type (R) correspond to products of reflections in hyperplanes $x_i = x_{i+1}$. The operation (X) corresponds to reflecting the vertex c to the origin (and the origin to c). It is indicated by the letter X because the corresponding matrix operation can also be interpreted as taking the logical *exclusive-or* operation between a fixed column and the remaining ones.

2.2 Dihedral angles of 0/1-simplices

Given a vertex v of a simplex $S \in \mathbb{S}^n$, the convex hull of the remaining vertices of S is the *facet* F_v of S opposite v . The *dihedral* angle α between two given facets of S is the angle supplementary to the angle γ between two normal vectors to those facets, both pointing into S or both pointing out of S . In other words, $\alpha + \gamma = \pi$.

Definition 2.5 A simplex $S \in \mathbb{S}^n$ will be called *nonobtuse* if none of its dihedral angles is obtuse (greater than $\pi/2$), and *acute* if all its dihedral angles are acute (less than $\pi/2$).

If P is a matrix representation of S with columns p_1, \dots, p_n , then the columns q_1, \dots, q_n of the matrix $Q = P^{-\top}$ are inward normals to the facets F_{p_1}, \dots, F_{p_n} , respectively, as $Q^\top P = I$. The vector q satisfying $P^\top q = e^n$ is orthogonal to each difference of two columns of P . It is an outward normal to the facet F_{p_0} opposite the origin p_0 and equals $q = P^{-\top} e^n = q_1 + \dots + q_n$. This proves the following proposition.

Proposition 2.6 ([4, 7]) *Let F_1, \dots, F_n be the facets of $S \in \mathbb{S}^n$ meeting at the origin and F_0 its facet opposite the origin, and let P be a matrix representation of S . Then F_0 makes nonobtuse dihedral angles with F_1, \dots, F_n if and only if for all $i \in \{1, \dots, n\}$,*

$$(e_i^n)^\top (P^\top P)^{-1} e^n \geq 0. \quad (7)$$

Moreover, each pair of facets F_i and F_j with $i \neq 0 \neq j$ makes a nonobtuse dihedral angle if and only if

$$(e_i^n)^\top (P^\top P)^{-1} e_j^n \leq 0, \quad (8)$$

for all $i, j \in \{1, \dots, n\}$. Therefore, S is nonobtuse if and only if both (7) and (8) hold.

Property (7) translates as *diagonal dominance* of $(P^\top P)^{-1}$, and (8) is called the *Stieltjes property* of $(P^\top P)^{-1}$, which is then called a *Stieltjes matrix*.

Remark 2.7 Condition (7) is equivalent with the statement that the vertex v of S at the origin orthogonally projects onto its opposite facet F_v . This proves that the following four statements are equivalent:

- S is nonobtuse;
- each vertex v of S projects orthogonally onto its opposite facet F_v ;
- each matrix representation P of S satisfies $(P^\top P)^{-1} e^n \geq 0$;
- each matrix representation P of S satisfies $(e_i^n)^\top (P^\top P)^{-1} e_j^n \leq 0$ for all $i, j \in \{1, \dots, n\}$.

In fact, the second and third condition in Remark 2.7 can be slightly relaxed. See Figure 4.

For each $j \in \{0, 1, 2, 3\}$, let P_j be a matrix representations of a tetrahedron $S \in \mathbb{S}^3$ with its vertex v_j located at the origin. If for instance $(P_j^\top P_j)^{-1} e^n \geq 0$ for $j \in \{1, 2, 3\}$ then F_1, F_2 and F_3 make only nonobtuse dihedral angles. These include *all* the six dihedral angles of S .

Remark 2.8 To characterize acute simplices similarly, replace \geq in (7) by $>$ and \leq in (8) by $<$. Moreover, replace *onto* by *into the interior* of its opposite facet.

The following two simple combinatorial lemmas will be used further on in this paper.

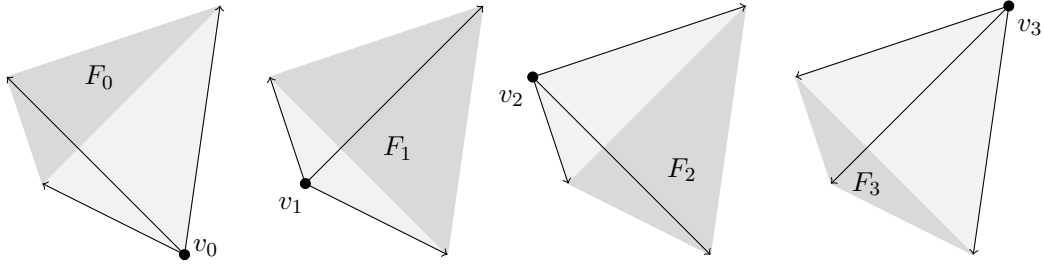


Figure 4: Dihedral angles are present in different ways in different matrix representations.

Lemma 2.9 *Let $P \in \mathbb{B}^{n \times n}$ represent a nonobtuse 0/1-simplex S . Then for all $v \in \mathbb{B}^n$,*

$$v^\top (P^\top P)^{-1} \bar{v} \leq 0. \quad (9)$$

If S is even acute then

$$v^\top (P^\top P)^{-1} \bar{v} < 0 \quad (10)$$

for all $v \in \mathbb{B}^n$ with $v \notin \{0, e^n\}$.

Proof. In fact, $v^\top (P^\top P)^{-1} \bar{v}$ is the sum of $\mathbf{1}(v)\mathbf{1}(\bar{v})$ of the off-diagonal entries of $(P^\top P)^{-1}$. According to Proposition 2.6 these are nonpositive if S is nonobtuse. According to Remark 2.8 they are negative if S is acute. \square

Lemma 2.10 *Let $P \in \mathbb{B}^{n \times n}$ represent a nonobtuse 0/1-simplex S . If for some $v \in \mathbb{B}^n$,*

$$v^\top (P^\top P)^{-1} \bar{v} = 0, \quad (11)$$

then $v = 0$ or $\bar{v} = 0$ or $P^\top P$ is reducible.

Proof. Let $v \neq 0 \neq \bar{v}$ and write $k = \mathbf{0}(v)$. Then $1 \leq k \leq n-1$. Let Π be a permutation such that $\text{supp}(\Pi \bar{v}) = \{1, \dots, k\}$. Writing $w = \Pi v$, we have that $\bar{w} = \Pi \bar{v}$ and

$$0 = v^\top (P^\top P)^{-1} \bar{v} = v^\top \Pi^\top \Pi (P^\top P)^{-1} \Pi^\top \Pi \bar{v} = w^\top \Pi (P^\top P)^{-1} \Pi^\top \bar{w}, \quad (12)$$

which is the sum of the entries of $\Pi (P^\top P)^{-1} \Pi^\top$ with indices (i, j) with $k+1 \leq i \leq n$ and $1 \leq j \leq k$. Since these entries are non-positive and their sum equals zero, they are all zero, leading to an $(n-k) \times k$ bottom left block of zeros in $\Pi (P^\top P)^{-1} \Pi^\top$. Thus, $(P^\top P)^{-1}$ is reducible, and hence, so is its inverse $P^\top P$. \square

A final important observation is the following classical result by Fiedler.

Lemma 2.11 ([13]) *All k -facets of a nonobtuse simplex are nonobtuse and all k -facets of an acute simplex are acute.*

It is well known that the converse does not hold. Simplices whose facets are all nonobtuse or acute were studied recently in [4].

3 Doubly stochastic patterns and full indecomposability

We start our investigations with some results on matrix representations of acute 0/1-simplices. The first one gives a remarkable connection with doubly stochastic matrices. It follows from the observation in Remark 2.7 that for an acute 0/1-simplex, the altitude from each vertex points into the interior of I^n . This, in turn, defines the signs of the entries of the normals to its facets in terms of the supports of their corresponding vertices.

Theorem 3.1 *Let $P \in \mathbb{B}^{n \times n}$ be a matrix representation of an acute 0/1-simplex $S \in \mathbb{S}^n$, and write $Q = P^{-\top}$. Then*

$$q_{ij} > 0 \Leftrightarrow p_{ij} = 1 \quad \text{and} \quad q_{ij} < 0 \Leftrightarrow p_{ij} = 0. \quad (13)$$

Defining $0 \leq C = (c_{ij})$ and $0 \leq D = (d_{ij})$ by

$$C = \frac{1}{2}(|Q| - Q) \quad \text{and} \quad D = \frac{1}{2}(|Q| + Q), \quad (14)$$

where $|Q|$ is the matrix whose entries are the moduli of the entries of Q , we have that

$$Q = D - C, \quad (15)$$

where D is doubly stochastic and C row-substochastic.

Proof. The j th column q_j of Q is an inward normal to the facet F_j of S opposite the j th column p_j of P . Thus, $p_j - \alpha q_j$ is an element of the interior of I^n for $\alpha > 0$ small enough. From this, (13) immediately follows. Combining this with the fact that the inner product between p_j and q_j equals one, the positive elements in each column of Q add to one. But since $Q^\top P = I$, also the inner products between corresponding rows of P and Q equals one, and thus also the positive elements in each row of Q add to one. Finally, Qe^n is the outward normal to the facet of S opposite the origin and thus it points into the interior of I^n . Consequently, $Qe^n > 0$, hence $De^n > Ce^n \geq 0$, which shows that C is row-substochastic. \square

Remark 3.2 For $n \geq 7$ there exist matrix representations $P \in \mathbb{B}^{n \times n}$ of acute 0/1-simplices in I^n for which the matrix C in (14) is not column-substochastic. This shows that Theorem 3.1 cannot be strengthened in this direction. It also proves that if P represents an acute 0/1-simplex, its transpose P^\top may not do the same. See Figure 5 for an example.

Corollary 3.3 *Let $P \in \mathbb{B}^{n \times n}$ be a matrix representation of an acute 0/1-simplex $S \in \mathbb{S}^n$. Then P has a fully indecomposable doubly stochastic pattern.*

Proof. Due to (13), the matrix D in (14) has the same support as P , hence P has a doubly stochastic pattern. Next, assume to the contrary that P is partly decomposable, then there exist permutations Π_1, Π_2 such that

$$\Pi_1^\top P \Pi_2 = \begin{bmatrix} P_{11} & P_{12} \\ 0 & P_{22} \end{bmatrix},$$

where P_{11} is a $k \times k$ matrix and P_{22} an $(n - k) \times (n - k)$ matrix for some $k \in \{1, \dots, n - 1\}$. But then $Q = P^{-\top}$ has entries equal to zero, which contradicts (13) in Theorem 3.1. \square

Theorem 3.1, Corollary 3.3, and Remark 3.2 are all illustrated in Figure 5.

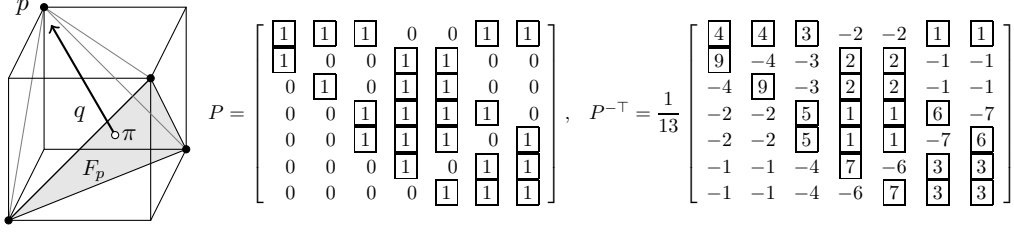


Figure 5: In an acute 0/1-simplex, each vertex p following the inward normal q to its opposite facet F_p (in converse direction) projects as π in the interior of F_p and hence in the interior of I^n . This fixes the signs of the entries of q in terms of those of p . The matrices P and $P^{-\top}$ (not related to the depicted tetrahedron) constitute an example of the linear algebraic consequences. The positions of the positive entries (boxed) of $P^{-\top}$ and P coincide. The positive part D of $P^{-\top}$ is doubly-stochastic. The negated negative part C of $P^{-\top}$ is a row-substochastic. It is not column-substochastic because the third column of C adds to $\frac{14}{13}$. Thus, even though also P^\top has a doubly stochastic pattern and is fully indecomposable, it is not a matrix representation of an acute binary simplex.

Remark 3.4 Because *each* matrix representation P of an acute 0/1-simplex has a fully indecomposable doubly stochastic pattern, applying to such a matrix P any operation of type (X), as described below Figure 3, results in another matrix with a fully indecomposable doubly stochastic pattern. From the linear algebraic point of view, this is remarkable because generally, both the 0/1-matrix properties of full indecomposability and of having a doubly stochastic pattern are destroyed under operations of type (X). See for instance

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \xrightarrow{(X)} \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \xrightarrow{(X)} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (16)$$

From the geometric point of view, this is easy to understand, as the fact that each altitude from each vertex of S points into the interior of I^n is invariant under the action of \mathcal{B}_n .

The geometric translation of Corollary 3.3 is that if $S \in \mathbb{S}^n$ is acute, none of its k -dimensional facets is contained in a k -dimensional facet of I^n for $k \in \{1, \dots, n-1\}$. The geometric *proof* of this is to note that, given a k -facet C of I^n , no vertex of I^n orthogonally projects into *the interior* of C . In fact, each vertex of I^n projects on a *vertex* of C . See Figure 6. Thus, if an arbitrary 0/1-simplex S has a k -facet K contained in C , each remaining vertex of S projects on a vertex of C . Remark 2.8 now shows that S cannot be acute.

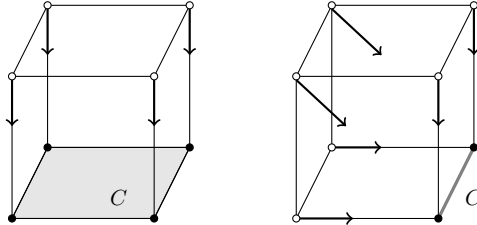


Figure 6: For each facet C of I^n , each vertex of I^n projects onto a vertex of C . Consequently, no acute 0/1-simplex has a facet contained in a facet of I^n .

Contrary to an acute 0/1-simplex, a *nonobtuse* 0/1-simplex S may indeed have a k -facet K that is contained in a cube facet C of I^n . If this is the case, then each remaining vertex of S projects on a vertex of K . Moreover, S has a partly decomposable matrix representation. Before discussing this structure, we first formulate the equivalent of Theorem 3.1 for nonobtuse simplices and discuss some of the differences with Theorem 3.1 using an example.

Theorem 3.5 *Let $P \in \mathbb{B}^{n \times n}$ be a matrix representation of a nonobtuse 0/1-simplex $S \in \mathbb{S}^n$, and write $Q = P^{-\top}$. Then*

$$q_{ij} \geq 0 \Leftrightarrow p_{ij} = 1 \quad \text{and} \quad q_{ij} \leq 0 \Leftrightarrow p_{ij} = 0. \quad (17)$$

Defining $0 \leq C = (c_{ij})$ and $0 \leq D = (d_{ij})$ by

$$C = \frac{1}{2}(|Q| - Q) \quad \text{and} \quad D = \frac{1}{2}(|Q| + Q), \quad (18)$$

where $|Q|$ is the matrix whose entries are the moduli of the entries of Q , we have that

$$Q = D - C, \quad (19)$$

where D is doubly stochastic and C row-substochastic.

Proof. The proof only differs from the proof of Theorem 3.1 in the sense that $p_j - \alpha q_j$ is now an element of I^n including its boundary. This accounts for the \geq and \leq signs in (17) in comparison to the $>$ and $<$ signs in (13). \square

Theorem 3.5 is rather weaker than Theorem 3.1. First of all, the matrix $P^{-\top}$ can have entries equal to zero. Moreover, it cannot anymore be concluded that P has a doubly stochastic pattern, only that it *contains* a doubly stochastic pattern,

$$\text{supp}(D) \subset \text{supp}(P). \quad (20)$$

A typical example of this is the following matrix representation P of a nonobtuse 0/1-simplex,

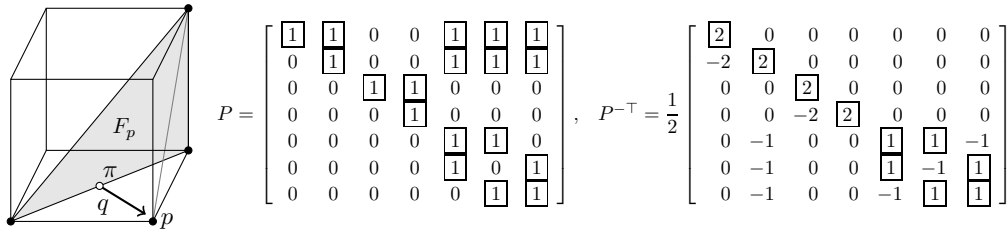


Figure 7: Analogue of Figure 5 for matrix representations of nonobtuse 0/1-simplices.

Obviously, P is partly decomposable and has no doubly stochastic pattern. It is only valid that the support of the doubly stochastic matrix D is *contained* in the support of P .

4 Partly decomposable matrix representations

We will continue to study nonobtuse 0/1-simplices having a partly decomposable matrix representation P . Without loss of generality, we may assume that P is nontrivially block partitioned as

$$P = \left[\begin{array}{c|c} N & R \\ \hline 0 & A \end{array} \right], \quad (21)$$

and that A is fully indecomposable.

Theorem 4.1 *Let $S \in \mathbb{S}^n$ be nonobtuse with a matrix representation P as in (21) with $N \in \mathbb{B}^{k \times k}$ with $k \in \{1, \dots, n-1\}$ and with A fully indecomposable. Then:*

- N is a matrix representation of a nonobtuse simplex in I^k ;
- A is a matrix representation of a nonobtuse simplex in I^{n-k} ;
- $R = \nu(e^k)^\top$, where $\nu = 0$ or ν is a column of N .

Proof. Lemma 2.11 proves that the first k columns of P together with the origin form a nonobtuse k -simplex, and obviously its vertices all lie in a k -facet of I^n . This proves the first item in the list of statements. Next, we compute

$$P^{-\top} = \left[\begin{array}{cc} N^{-\top} & 0 \\ -A^{-\top}R^\top N^{-\top} & A^{-\top} \end{array} \right]. \quad (22)$$

and thus,

$$(P^\top P)^{-1} = \left[\begin{array}{cc} (N^\top N)^{-1} + N^{-1}R(A^\top A)^{-1}R^\top N^{-\top} & -N^{-1}R(A^\top A)^{-1} \\ -(A^\top A)^{-1}R^\top N^{-\top} & (A^\top A)^{-1} \end{array} \right]. \quad (23)$$

Due to Proposition 2.6, the matrix $(P^\top P)^{-1}$ has nonpositive off-diagonal entries (8) and nonnegative row sums (7). Both properties are clearly inherited by its trailing submatrix $(A^\top A)^{-1}$, possibly even with larger row sums. This proves the second statement of the theorem. Next, due to (8), the top-right block in (23) satisfies

$$-N^{-1}R(A^\top A)^{-1} \leq 0. \quad (24)$$

Multiplication of this block from the left with $N \geq 0$ and from the right with $\bar{R} \geq 0$ gives that

$$R(A^\top A)^{-1}\bar{R}^\top \geq 0. \quad (25)$$

However, by Lemma 2.9, the diagonal entries of $R(A^\top A)^{-1}\bar{R}^\top$ are also nonpositive, and thus, they all equal zero. We can therefore apply Lemma 2.10. Note that because A is assumed fully indecomposable, $A^\top A$ is irreducible by Lemma 2.3. Thus, row-by-row application of Lemma 2.10 proves that each row of R contains only zeros or only ones. This proves that there exists an $r \in \mathbb{B}^n$ such that

$$R = r(e^{n-k})^\top. \quad (26)$$

We will proceed to show that r is a column of N , or zero. Substituting (26) back into (24) yields that

$$wu^\top \geq 0, \quad \text{where } w = N^{-1}r \quad \text{and} \quad u^\top = (e^{n-k})^\top (A^\top A)^{-1}. \quad (27)$$

Due to (7) we have $u \geq 0$. Because $A^\top A$ is non-singular, u has at least one positive entry. Thus, also w is nonnegative. This turns $r = Nw$ into a nonnegative linear combination of columns of N . We continue to prove that it is a *convex* combination. For this, observe that the sums of the last k rows of $(P^\top P)^{-1}$ are nonnegative due to (7). Thus,

$$0 \leq -(A^\top A)^{-1} R^\top N^{-\top} e^k + (A^\top A)^{-1} e^{n-k} = u \left(1 - w^\top e^k \right)$$

with u, w as in (27) and where we have used that $R^\top N^{-\top} = e^{n-k} r^\top N^{-\top} = e^{n-k} w^\top$. As we showed already that $u \geq 0$ has at least one positive entry, we conclude that

$$w^\top e^k \leq 1.$$

Therefore we now have that $Nw = r \in \mathbb{B}^k$ for some $w \geq 0$ with $w^\top e^k \leq 1$. Thus also

$$[0 \mid N] \begin{bmatrix} 1 - w^\top e^k \\ w \end{bmatrix} = r. \quad (28)$$

According to Lemma 2.4, this implies that r is a column of $[0 \mid N]$. This proves the third item in the list of statements to prove. \square

It is worthwhile to stress a number of facts concerning Theorem 4.1 and its nontrivial proof.

Remark 4.2 The assumption that A in (21) is fully indecomposable is very natural, as each partly decomposable matrix can be put in the form (21) using operations of type (C) and (R). But in the proof of Theorem 4.1 we only needed that $A^\top A$ is irreducible. This is *implied* by the full indecomposability of A due to Lemma 2.3, but is not *equivalent* to it. In fact, if A is fully indecomposable, then $A^\top A \geq e^n (e^n)^\top + I$. See Corollary 6.5.

Remark 4.3 The result proved in the third bullet of Theorem 4.1 that R consists of $n - k$ copies of *the same* column of N is stronger than the geometrical observation that each of the last $n - k$ columns of P should project on *any* vertex of the k -simplex represented by N . It is the *irreducibility* of $A^\top A$ that forces the equality of all columns of R .

Remark 4.4 Permuting rows and columns of the block upper triangular matrix in (21) show that also for

$$\left[\begin{array}{c|c} A & 0 \\ \hline R & N \end{array} \right] \quad (29)$$

with A and N as in Theorem 4.1, similar conclusions can be drawn for R .

Some details in the above remarks will turn out to be of central importance in Section 6.

Corollary 4.5 *Let $S \in \mathbb{S}^n$ be a nonobtuse 0/1-simplex with matrix representation P . Then the following statements are equivalent:*

- P is partly decomposable;
- S has a block diagonal matrix representation with at least one fully indecomposable block;
- each matrix representation of S is partly decomposable.

Proof. Suppose that P is partly decomposable. Then Theorem 3.1 shows that P is of the form

$$P = \left[\begin{array}{c|c} N & \nu (e^{n-k})^\top \\ \hline 0 & A \end{array} \right], \quad (30)$$

and $\nu = 0$ or ν is a column of N . If $\nu = 0$ then P itself is block diagonal. If $\nu \neq 0$, apply to P the operation of type (X) as described below Figure 3 with column c equal to the column $(\nu, 0)^\top$ of P . The simple observation that $\nu + \nu$ equal zero modulo 2 proves that the resulting matrix \tilde{P} is block diagonal. As the bottom right block of \tilde{P} equals A , this shows that at least one block is fully indecomposable. To show that each matrix representation of S is partly decomposable, simply note that each operation of type (X) applied to the block-diagonal matrix representation will leave one of the two off-diagonal zero blocks invariant. \square

Remark 4.6 The converse of Theorem 4.1 is also valid. Indeed, suppose that N and A are matrix representations of nonobtuse simplices. Then it is trivially true that the block diagonal matrix P having N and A as diagonal blocks represents a nonobtuse simplex. Applying operations of type (X) to P proves that all matrices of the form (30) then represent nonobtuse simplices. Note that this also holds without the assumption that A is fully indecomposable.

Another corollary of Theorem 4.1 concerns its implications for the structure of the transposed inverse $P^{-\top}$ of a partly decomposable matrix representation of a nonobtuse 0/1-simplex.

Corollary 4.7 *If $\nu = Ne_j^k$ in (30) for some $j \in \{1, \dots, k\}$, then*

$$P^{-\top} = \left[\begin{array}{c|c} N^{-\top} & 0 \\ \hline ae_j^\top & A^{-\top} \end{array} \right], \quad (31)$$

where a is the inward normal to the facet opposite the origin of the simplex represented by A . As a consequence, the sums of the last $n - k$ rows of $P^{-\top}$ all add to zero.

Proof. Substitute $R = \nu e^{n-k}$ with $\nu = Ne_j^k$ into the expression for $P^{-\top}$ in (22). \square

To illustrate Corollary 4.5, consider again the matrix $P \in \mathbb{B}^{7 \times 7}$ from Figure 7, now displayed not as 0/1-matrix but as checkerboard black-white pattern, at the top in Figure 8. Applying an operation of type (X) with the second column results in the matrix to its right, which is block diagonal. Swapping the first two rows of that matrix yields one in which the top left block is now in its most reduced form. Applying an operation of type (X) with the sixth column results in a matrix in which the bottom left 3×4 zero block has been destroyed. Finally, swapping columns 2 and 6, and swapping rows 1 and 2, results in the matrix that could also have been obtained by applying operation (X) with column 6 directly to P .

Corollary 4.5 shows that the matrix representations of a nonobtuse 0/1-simplex are either all partly decomposable, or all fully indecomposable. This motivates the following definition.

Definition 4.8 A nonobtuse simplex is called partly decomposable if it has a partly decomposable matrix representation, and fully indecomposable if it has not.

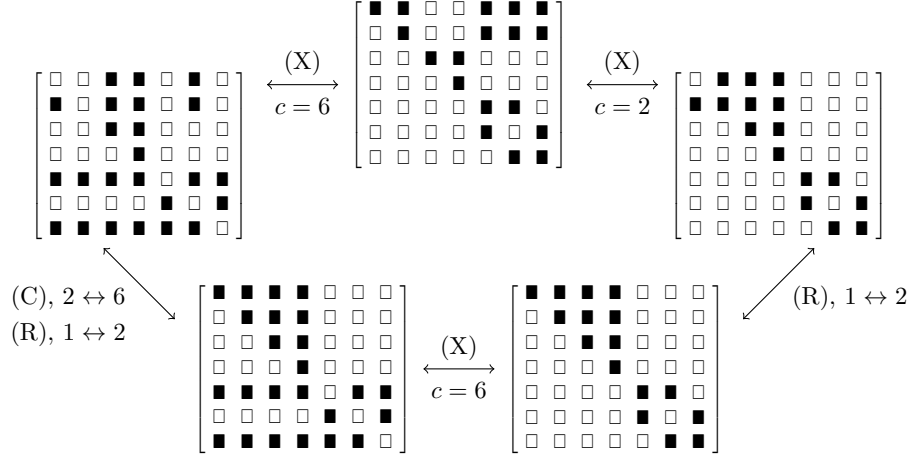


Figure 8: Illustration of Corollary 4.5 using the matrix $P \in \mathbb{B}^{7 \times 7}$ from Figure 7.

We will now investigate to what structure the recursive application of Theorem 4.1 leads. For this, assume again that P is a partly decomposable matrix representation of a nonobtuse 0/1-simplex $S \in \mathbb{S}^n$. Then by Corollary 4.5, S has a matrix representation of the form

$$P = \left[\begin{array}{c|c} N_1 & R_1 \\ \hline 0 & A_1 \end{array} \right], \quad (32)$$

in which A_1 is fully indecomposable. According to Theorem 4.1, the $k \times k$ matrix N_1 represents a nonobtuse k -simplex K in I^k . If also K is partly decomposable, we can block-partition N_1 using row (R) and column (C) permutations Π_1 and Π_2 , such that

$$\tilde{P} = \Pi_1 P \Pi_2 = \left[\begin{array}{c|c|c} N_2 & R_{12} & R_{13} \\ \hline 0 & A_2 & R_{23} \\ \hline 0 & 0 & A_1 \end{array} \right], \quad (33)$$

with A_2 fully indecomposable and N_2 possibly partly decomposable. Theorem 4.1 shows that

$$R_{12} \text{ consists of copies of a column } \nu \text{ of } [0|N_2],$$

and

$$\left[\begin{array}{c} R_{13} \\ R_{23} \end{array} \right] \text{ consists of copies of a column of } \left[\begin{array}{c|c} N_2 & R_{12} \\ \hline 0 & A_2 \end{array} \right].$$

This means that if R_{23} is nonzero, then R_{13} consists of copies of the same column ν of N as does R_{12} . Thus the whole block $[R_{12} | R_{23}]$ consists of copies of a column ν of $[0|N_2]$. On the other hand, if R_{23} is zero, then R_{13} can either be zero, or consist of copies of *any* column of N_2 , including ν .

By including operations of type (X) it is possible to map the entire strip above one of the fully indecomposable diagonal blocks to zero. Although this will in general destroy the block upper triangular form of the square submatrix to the left of that strip, Corollary 4.7 shows that this submatrix remains partly decomposable. Therefore, its block upper triangular structure can be restored using only operations of type (R) and (C), which leave the zero strip intact.

Remark 4.9 It is generally not possible to transform \tilde{P} to block diagonal form with more than two diagonal blocks. See the tetrahedron S in I^3 in Figure 9. It is possible to put a vertex of S at the origin such that facets A and N are orthogonal, and hence the corresponding matrix representation is block diagonal with two blocks. The triangular facet however requires a *different* vertex at the origin for its 2×2 matrix representation to be diagonal.

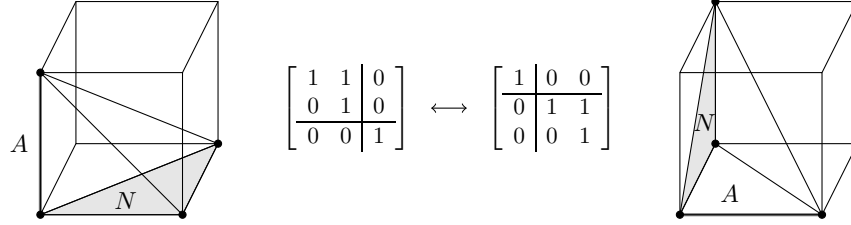


Figure 9: Any simplex S with a partly decomposable matrix representation has a pair of facets A and N of dimensions adding to n are orthogonal to one another.

Summarizing, the above discussion shows that each nonobtuse 0/1-simplex S has a matrix representation that is block upper triangular, with fully indecomposable diagonal blocks (possibly only one). The strip above each diagonal block is of rank one and consists only of copies of a column to the left of the strip. Any matrix representation P of S can be brought into this form using only operations of type (C) and (R). Using an additional reflection of type (X), it is possible to transform an entire strip above one of the diagonal blocks to zero using a column to the left of the strip. Although this may destroy the block upper triangular form to the left of the strip, this form can be restored using operations of type (R) and (C) only.

In view of Corollary 4.7, the transposed inverse $P^{-\top}$ of a partly decomposable matrix representation P of a nonobtuse 0/1-simplex S is perhaps even simpler in structure than P itself. On the diagonal it has the transposed inverses of the fully indecomposable diagonal blocks A_1, \dots, A_p of P , and each *horizontal* strip to the left of such a diagonal block $(A_j)^{-\top}$ has *at most* one nonpositive column that is not identically zero. This column has two interesting features. The first is that it nullifies the sums of the rows in its strip. The second is that its position clearly indicates to which vertex of which other block A_i the block A_j is related. To illustrate what we mean by this, see Figure 7 for an example. Above the bottom right 3×3 block A of P we see copies of the second column of P . This fact can also be read from the position of the nonzero entries to the left of the corresponding block $A^{-\top}$ in $P^{-\top}$.

Remark 4.10 The above shows that to each nonobtuse 0/1-simplex S of dimension n we can associate a special type of simplicial complex C_p consisting of p mutually orthogonal fully indecomposable simplicial facets S_1, \dots, S_p with respective dimensions k_1, \dots, k_p adding to n , where each facet S_j lies in its own k_j -facet of I^n . Explicitly, let $C_1 = S_1$. The complex C_{j+1} is obtained by attaching a vertex of S_{j+1} to a vertex v of C_j , such that the orthogonal projection of S_{j+1} onto the $(k_1 + \dots + k_j)$ -dimensional ambient space of C_j equals v .

Remark 4.10 is illustrated by the tetrahedron in Figure 9. It can be built from three 1-simplices S_1, S_2, S_3 simply by first attaching S_2 with a vertex to a vertex of S_1 orthogonally to S_1 , giving

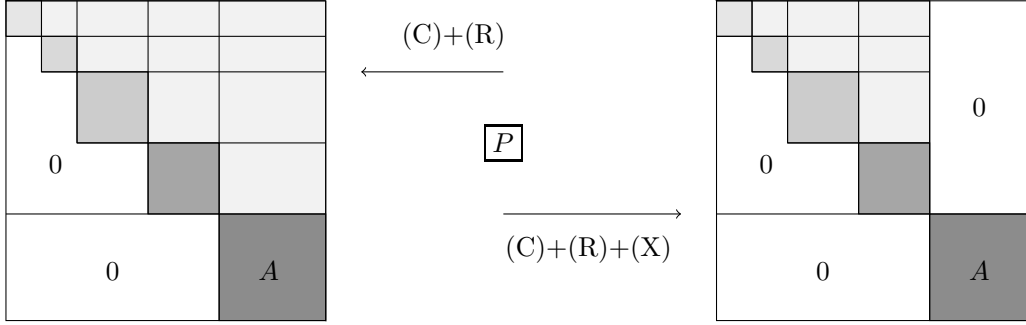


Figure 10: A partly decomposable matrix representation P of a nonobtuse 0/1-simplex S can be brought in the left form using operations of type (C) and (R) only, and in the right form if using additional operations of type (X). The diagonal blocks are fully indecomposable.

a right triangle C_2 . Then attaching S_3 to the correct vertex v of C_2 such that the projection of S_3 onto C_2 equals v gives the tetrahedron. In Section 5 we will pay special attention to the nonobtuse simplices whose fully indecomposable components are n -cube edges.

Remark 4.11 The 1-simplex in I^n has a fully indecomposable matrix representation with doubly stochastic pattern. It is formally an acute simplex. Indeed, the normals to its 0-dimensional facets 0 and 1 point in opposite directions. Hence, its only dihedral angle equals zero. Since there does not exist a fully indecomposable triangle in I^2 , matrix representations of a partly decomposable simplex do not have 2×2 fully indecomposable diagonal blocks.

We would like to stress that although each partly decomposable matrix representation of a nonobtuse 0/1-simplex can be transformed into block diagonal form by operations of types (C),(R) and (X) as depicted in the right in Figure 10, the bottom right block cannot be *any* of the fully indecomposable diagonal blocks A_j . This is only possible if the corresponding simplex S_j is attached to the remainder of the complex at exactly one vertex. For example, in Figure 11, with 0 as the origin, the matrix A_3 representing a regular tetrahedron in I^3 is a block of a block diagonal matrix. After mapping vertex 4 to the origin with a reflection of type (X), the block A_4 representing a so-called antipodal 4-simplex in I^4 is. However, the block A_2 representing the 1-simplex in I^1 is never a block of a block diagonal matrix representation of S . The only configurations of the three building blocks S_1, S_2, S_3 having a matrix representation that can be transformed by operations of type (C),(R) and (X) onto block diagonal form with three diagonal blocks, are those in which S_1, S_2 and S_3 have a common vertex.

In general, the decomposability structure of a nonobtuse 0/1-simplex can be well visualized as a special type of planar graph, at the cost of the geometrical structure. For this, assign to each $p \times p$ fully indecomposable diagonal block a regular p -gon, and to attach these to one another at the common vertex of the simplices they represent. See Figure 12 for an example. At the white vertices it is indicated how many p -gons meet. This number equals the number of diagonal blocks in the matrix representation when this vertex is reflected onto the origin.

Before studying further properties of partly decomposable nonobtuse 0/1-simplices in terms of their fully indecomposable components, we will pay special attention to *orthogonal* simplices.

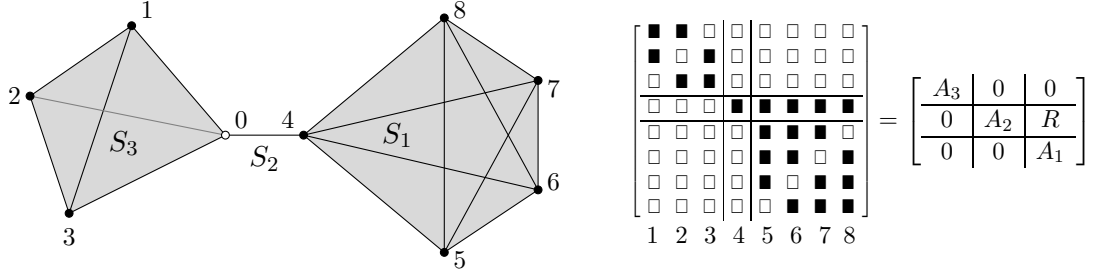


Figure 11: A simplicial complex of three mutually orthogonal simplices S_1, S_2, S_3 . The given matrix representation corresponds to choosing the vertex 0 as the origin. Reflecting vertex 4 to the origin decouples, alternatively, the bottom right 4×4 block. It is not possible to transform the matrix to block diagonal form with $A_2 = [1]$ as one of the diagonal blocks. Reflecting any other vertex to the origin does not even lead to a block diagonal matrix representation.

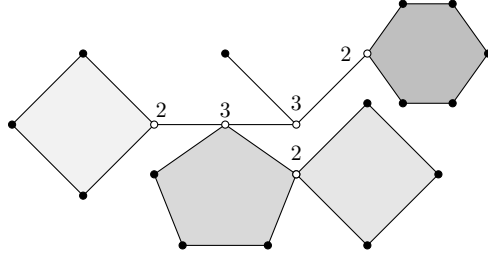


Figure 12: Schematic representation of a simplicial complex, built from a 5-simplex, a 4-simplex, two tetrahedra, and four edges, of total dimension 19. With the origin at a white vertex, the matrix representation decouples into the indicated number of diagonal blocks. If the vertex is located at another vertex, the matrix representation does not decouple.

5 Orthogonal simplices and their matrix representations

The simplest class of nonobtuse simplices is formed by the *orthogonal simplices*. These are nonobtuse simplices with $\binom{n}{2} - n$ right dihedral angles. Note that this is the *maximum* number of right dihedral angles a simplex can have, as Fiedler proved in [13] that any simplex has at least n acute dihedral angles. Orthogonal simplices are useful in many applications, see [6, 9] and the references therein. We will restrict our attention to orthogonal 0/1-simplices.

The orthogonal 0/1-simplices can be defined recursively as follows [6]. The cube edge I^1 is an orthogonal simplex. Now, a nonobtuse 0/1-simplex S in I^n is orthogonal if it has an $(n-1)$ -facet F with the properties that:

- F is contained in an $(n-1)$ -facet of I^n ;
- F is an orthogonal $(n-1)$ -simplex.

Clearly, this way to construct orthogonal 0/1-simplices is a special case of how nonobtuse 0/1-simplices were constructed from their fully indecomposable parts in Section 4. This is because a vertex v forms an orthogonal simplex S together with an $(n-1)$ -facet F that is contained in an $(n-1)$ -facet of I^n if and only if v projects orthogonally on a vertex of F . This

shows in particular that all fully indecomposable components of any matrix representation of S equal $[1]$, which limits the number of their upper triangular matrix representations.

Proposition 5.1 *There exist $n!$ distinct upper triangular 0/1 matrices that represent orthogonal 0/1-simplices in I^n .*

Proof. Let $P \in \mathbb{B}^{n \times n}$ be an upper triangular matrix representing an orthogonal n -simplex. Then the matrix

$$\tilde{P} = \left[\begin{array}{c|c} P & r \\ \hline 0 & 1 \end{array} \right]$$

is upper triangular, and according to Theorem 4.1 it represents a nonobtuse simplex if and only if r equals one of the $n+1$ distinct columns of $[0 | P]$. Thus there are $n+1$ times as many matrix representations of orthogonal $(n+1)$ -simplices in I^{n+1} as of orthogonal n -simplices in I^n , whereas $[1]$ is the only one in I^1 . \square

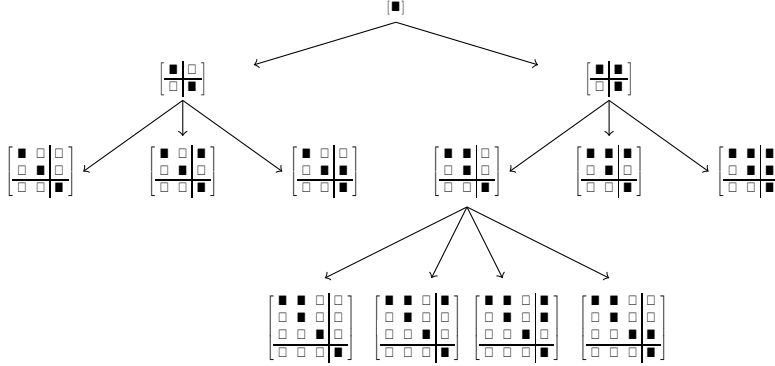


Figure 13: There are $n!$ upper triangular matrix representations of orthogonal 0/1-simplices.

Remark 5.2 Modulo the action of the hyperoctahedral group, there remain as many as the number of unlabeled trees on $n+1$ vertices. Indeed, it is not hard to verify that two matrices P and R representing orthogonal 0/1-simplices can be transformed into one another using operations of type (R),(C) and (X) if and only if the spanning trees of orthogonal edges of the simplices corresponding to P and R are isomorphic as graphs.

6 One Neighbor Theorem for a class of nonobtuse simplices

In this section we will discuss the one neighbor theorem for acute simplices [6] and generalize it to a larger class of nonobtuse simplices. This appears a very nontrivial matter, which can be compared with the complications that arise when generalizing the Perron- Frobenius theory for positive matrices to nonnegative matrices [1, 2].

6.1 The acute case revisited

The one neighbor theorem for acute 0/1-simplices reads as follows. We present a alternative proof to the proof in [6], based in Theorem 3.1.

Theorem 6.1 (One Neighbor Theorem) *Let S be an acute 0/1-simplex in I^n , and F an $(n-1)$ -facet of S opposite the vertex v of S . Write \hat{S} for the convex hull of F and \bar{v} . Then:*

- F does not lie in an $(n-1)$ -facet of I^n ;
- \hat{S} is the only 0/1-simplex having F as a facet that may be acute, too.

In words, an acute 0/1-simplex has at most one acute face-to-face neighbor at each facet.

Proof. Let q be a normal vector to a facet of F opposite a vertex p of an acute 0/1-simplex S . Then due to Theorem 3.1, q has no zero entries. Therefore, the line $v + \alpha q$ parametrized by $\alpha \in \mathbb{R}$ intersect the interior of I^n if and only if $v \in \{p, \bar{p}\}$. Thus, for other vertices v of I^n , the altitude from v to the ambient hyperplane of F does not land in I^n and thus not in F . This is however a necessary condition for the convex hull of F and v to be acute. \square

See the left picture in Figure 14 for an illustration of Theorem 6.1 in I^3 . Only the pair of white vertices end up inside I^3 when following the normal direction q of the facet F . All six other vertices, when projected on the plane containing F end up outside I^3 , or on themselves.

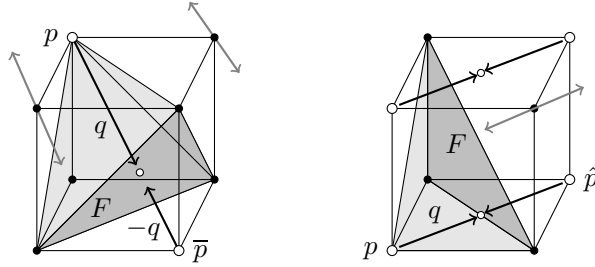


Figure 14: Left: for any facet F of an acute 0/1-simplex, there is only one pair of antipodal vertices p, \bar{p} that may project onto F . All others end up outside I^n when following the normal q in either direction. Right: in a nonobtuse simplex, there can be more than two vertices that remain in I^n when following the normal direction to an interior facet.

The translation of Theorem 6.1 in terms of linear algebra is as follows.

Corollary 6.2 *Let $P \in \mathbb{B}^{n \times (n-1)}$. The matrix $[P | v] \in \mathbb{B}^{n \times n}$ is a matrix representation of an acute 0/1-simplex for at most one pair of antipodal points $v \in \{p, \bar{p}\} \subset \mathbb{B}^n$.*

The one neighbor theorem dramatically restricts the number of 0/1-polytopes that can be face-to-face triangulated by acute simplices. For instance, only from dimension $n = 7$ onwards there exists a pair of face-to-face acute simplices in I^n . In I^7 it is the Hadamard regular simplex [14] and its face-to-face neighbor, which is unique modulo the action of the hyperoctahedral group, and which has the one-but- largest volume in I^7 over all acute 0/1-simplices [5]. Also in [6] the theorem turned out useful in constructing all possible face-to-face triangulations of I^n consisting on nonobtuse simplices only, due to the following sharpening of the statement.

Corollary 6.3 *Each acute 0/1-simplex S in I^n has at most one face-to-face nonobtuse neighbor at each of its facets.*

Proof. This follows from the fact that in the proof of Theorem 6.1, the altitudes from $v \neq \{p, \bar{p}\}$ intersect I^n only in v itself. \square

A natural question is what can be proved for nonobtuse-0/1 simplices. Theorem 3.5 showed that a normal to a facet of a nonobtuse 0/1-simplex S can have entries equal to zero. Writing $\mathbf{0}(q)$ for the number of entries of q equal to zero, there are $2^{\mathbf{0}(q)+1}$ vertices v of I^n from which the altitudes starting at v onto the plane containing F do not leave I^n . This is illustrated in the right picture in Figure 14. The normal vector q to the facet F has one zero entry: $\mathbf{0}(q) = 1$. The altitudes from the 2^2 white vertices of I^3 onto the plane containing F lie in I^3 .

Nevertheless, only the altitudes from p and \hat{p} land on F itself, and we see that the interior facet F of S in I^3 has exactly one nonobtuse neighbor. It is tempting to conjecture that the one neighbor theorem holds also for nonobtuse 0/1-simplices. The only adaption to make is then, based on the example in Figure 14, that instead of the antipodal \bar{p} of p in I^n , the second vertex \hat{p} such that the convex hull of F with \hat{p} is a nonobtuse simplex would satisfy

$$\hat{p}_j = 1 - p_j \Leftrightarrow q_j \neq 0 \text{ and } \hat{p}_j = 0 \Leftrightarrow q_j = 0. \quad (34)$$

In words, \hat{p} is the antipodal of p restricted to the $(n - \mathbf{0}(q))$ -dimensional n -cube facet that contains both p and q . In Figure 14, \hat{p} is the antipodal of p in the bottom square facet of I^3 .

As an attempt to prove this conjecture, one may try to demonstrate that the remaining white vertices in the top square facet of I^3 , although their altitudes lie in I^3 , cannot fall onto F . Although we did not succeed in doing so, the nonobtusity of S is a necessary condition. To see this, consider the 0/1-simplex S in I^5 with matrix representation

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix} \quad \text{with } q = \frac{1}{2} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad (35)$$

and q is the normal to the facet F of S opposite the origin. Observe that the line from the origin to the vertex $2q$ in I^5 intersects F in the midpoint of its edge between the two vertices of S in the last two columns of P . This shows that both the origin and its antipodal in the bottom 4-facet of I^5 as defined in (34) land in F when following their respective altitudes. But also the line between e_1^5 and e^5 intersects F in the midpoint of its edge between the two vertices in the first and third column of P . Thus, also both the vertices e_1^5 and e^5 in the top 4-facet of I^5 land in F when following their altitudes. Thus, for a 0/1-simplex that is not nonobtuse, it can occur that more than two vertices of I^n project orthogonally onto F .

6.2 More on fully indecomposable nonobtuse simplices

In Section 6.3 we will study the one neighbor theorem in the context of partly decomposable nonobtuse simplices. For this, but also for its own interest, we derive two auxiliary results on fully indecomposable nonobtuse simplices.

Lemma 6.4 *Each representation $P \in \mathbb{B}^{n \times n}$ of a fully indecomposable 0/1-simplex S satisfies*

$$P^\top P \geq I + e^n (e^n)^\top. \quad (36)$$

In geometric terms this implies that all triangular facets of S are acute.

Proof. A standard type of argument is the following. Write D for the diagonal matrix having the same diagonal entries as $B = (P^\top P)^{-1}$, and let $C = D - B$. Then $C \geq 0$, and

$$B = D - C = D(I - D^{-1}C) \quad \text{and} \quad P^\top P = B^{-1} = (I - D^{-1}C)^{-1}D^{-1}. \quad (37)$$

Because B is an M-matrix [16, 17], the spectral radius of $D^{-1}C$ is less than one, and the following Neumann series converges:

$$(I - D^{-1}C)^{-1} = \sum_{j=0}^{\infty} (D^{-1}C)^j. \quad (38)$$

Since P is fully indecomposable, $P^\top P$ is irreducible, and thus B is irreducible. But then, so are C and $D^{-1}C$. Because of the latter, for each pair k, ℓ there is a j such that $e_k^\top (D^{-1}C)^j e_\ell > 0$. This proves that $B^{-1} = P^\top P > 0$. Since its entries are integers, $P^\top P \geq e^n (e^n)^\top$. Thus, each pair of edges of S that meet at the origin makes an acute angle. As by Theorem 3.1 all matrix representations of S are fully indecomposable, we conclude that all triangular facets of S are acute. This implies that any diagonal entry of $P^\top P$ is greater than the remaining entries in the same row. Indeed, if two entries in the same row would be equal, then $p_j^\top (p_j - p_i) = 0$, which corresponds to two edges of S making a right angle. \square

Corollary 6.5 *Let P be a fully indecomposable matrix representation of a nonobtuse 0/1-simplex. If \hat{P} equals P with one column replaced by its antipodal, then $\hat{P}^\top \hat{P} > 0$.*

Proof. Without loss of generality, assume that

$$P = [p \mid P_1] \quad \text{and} \quad \hat{P} = [\bar{p} \mid P_1] \quad (39)$$

with $p \in \mathbb{B}^n$. Then

$$\hat{P}^\top \hat{P} = \begin{bmatrix} \bar{p}^\top \bar{p} & \bar{p}^\top P_1 \\ P_1^\top \bar{p} & P_1^\top P_1 \end{bmatrix}, \quad (40)$$

and $P_1^\top P_1 > 0$ because $P^\top P > 0$ as proved in Lemma 2.11. Due to the fact that for all $a, b \in \mathbb{B}^n$,

$$a^\top \bar{b} = a^\top (e^n - b) = a^\top (a - b), \quad (41)$$

we see that also $P_1^\top \bar{p} > 0$. Indeed, a zero entry would contradict that the diagonal entries of $P^\top P$ are greater than its off-diagonal entries, as proved in Lemma 6.4. \square

Remark 6.6 The matrix \hat{P} in Corollary 6.5 is not always fully indecomposable. See

$$P = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \hat{P} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad (42)$$

where the first columns of both matrices are each other's antipodal. This example also shows that the top left diagonal entry of $\hat{P}^\top \hat{P}$ need not be greater than the other entries in its row.

We end this section with a theorem which was proved by inspection of a finite number of cases. We refer to [5] for details on how to computationally generate the necessary data.

Theorem 6.7 *Each fully indecomposable nonobtuse 0/1-simplex in \mathbb{S}^n with $n \leq 8$ is acute. There exist fully indecomposable nonobtuse 0/1-simplices in \mathbb{S}^n with $n \geq 9$ that are not acute.*

Proof. See [5] for details on an algorithm to compute 0/1-matrix representations of 0/1-simplices modulo the action of the hyperoctahedral group. By inspection of all 0/1-simplices of dimensions less than or equal to 8, we conclude the first statement. For the second statement, we give an example. The 9×9 matrix in Figure 15 represents a nonobtuse simplex that is not acute, but P is fully indecomposable. \square

$$P = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}, \quad P^{-\top} = \frac{1}{20} \begin{bmatrix} 6 & 6 & -2 & -6 & 2 & 2 & 2 & 2 & -2 \\ 7 & -3 & 1 & 3 & 4 & -6 & -6 & 4 & 1 \\ 7 & -3 & 1 & 3 & -6 & 4 & 4 & -6 & 1 \\ -3 & 7 & 1 & 3 & 4 & -6 & 4 & -6 & 1 \\ -3 & 7 & 1 & 3 & -6 & 4 & -6 & 4 & 1 \\ -4 & -4 & 8 & 4 & 2 & 2 & 2 & 2 & -12 \\ -2 & -2 & 4 & -8 & 6 & 6 & -4 & -4 & 4 \\ -2 & -2 & 4 & -8 & -4 & -4 & 6 & 6 & 4 \\ -4 & -4 & -12 & 4 & 2 & 2 & 2 & 2 & 8 \end{bmatrix}, \quad \frac{1}{20} \begin{bmatrix} 10 \\ 5 \\ 5 \\ 5 \\ 5 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Figure 15: Example of a fully indecomposable matrix representation P of a nonobtuse simplex S that is not acute. The vector on the right is its normal q to the facet F opposite the origin. Since q has entries equal to zero, S cannot be acute. But $(P^\top P)^{-1}$ satisfies (7) and (8), hence S is nonobtuse. Note that none of the other normals has a zero entry.

Thus, Theorem 6.7 and Figure 14 prove that the *indecomposability* of a matrix representation of a nonobtuse 0/1-simplex S is, in fact, a *weaker* property than the *acuteness* of S .

Especially since the two concepts coincide up to dimension eight, this came as a surprise. Citing Günther Ziegler in Chapter 1 of *Lectures on 0/1-Polytopes* [18]: “*Low-dimensional intuition does not work!*”. See [5] for more such examples in the context of 0/1-simplices.

6.3 A One Neighbor Theorem for partly decomposable simplices

Let S be a partly decomposable nonobtuse simplex. Then according to Corollary 4.5, S has a matrix representation

$$P = \begin{bmatrix} N & 0 \\ 0 & A \end{bmatrix} \quad (43)$$

in which A is fully indecomposable. We will discuss some cases in which a modified version of the One Neighbor Theorem 6.1 holds also for nonobtuse simplices that are not acute.

Case I. To illustrate the main line of argumentation, consider first the simplest case, which is that $S \in \mathbb{S}^n$ can be represented by

$$P = \begin{bmatrix} A_2 & 0 \\ 0 & A_1 \end{bmatrix}, \quad \text{with } A_1 \in \mathbb{B}^{k \times k} \quad \text{and} \quad A_2 \in \mathbb{B}^{(n-k) \times (n-k)} \quad (44)$$

and in which A_1 and A_2 represent acute simplices S_1 and S_2 . Then A_1 and A_2 are fully indecomposable, and S_1 and S_2 satisfy the One Neighbor Theorem 6.1. Assume first that neither A_1 or A_2 equals the 1×1 matrix $[1]$.

Notation. We will write $X^j(y)$ for the matrix X with column j replaced by y .

Now, let $v \in \mathbb{B}^n$, partitioned as $v^\top = (v_1^\top \ v_2^\top)$ with $v_1 \in \mathbb{B}^k$. Assume that the block lower triangular matrix $P^1(v)$ represents a nonobtuse simplex. This implies that its top-left diagonal block $A_2^1(v_1)$ does so, too, hence $v_1 = a_1 = Ae_1^k$ or $v_1 = \overline{a_1}$ by Theorem 6.1. Corollary 6.5 shows that in both cases $A_2^1(v_1)^\top A_2^1(v_1) > 0$. But then Theorem 4.1 in combination with the observations in Remarks 4.2 and 4.4 proves that $v_2 = 0$, because all columns in the off-diagonal block must be copies of one and the same column of A_1 . Hence, there is at most one $v \in \mathbb{B}^n$ other than Pe_1^n such that $P^1(v)$ is nonobtuse. See Figure 16 for a sketch of the proof.

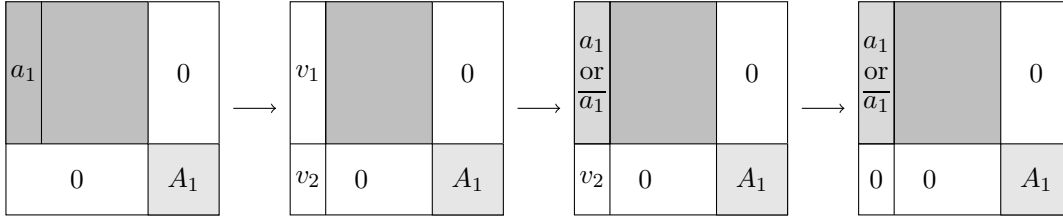


Figure 16: Steps in proving a one neighbor theorem for partly decomposable nonobtuse simplices with two fully indecomposable blocks representing acute simplices.

Clearly, the same argument can be applied to prove that for all $j \in \{1, \dots, n\}$, the matrix $P^j(v)$ represents a nonobtuse 0/1-simplex for at most one $v \in \mathbb{B}^n$ other than Pe_j^n . This proves that for each column p of P , the facet F_p of S opposite p has at most one nonobtuse neighbor. It remains to prove the same for the facet F_0 of S opposite the origin. But because S_1 and S_2 are by assumption acute, the normals q_1 and q_2 to their respective facets opposite the origin, which satisfy $A_1^\top q_1 = e_k^k$ and $A_2^\top q_2 = e_{n-k}^{n-k}$, are both positive. But then so is the normal q of F_0 , which satisfies $P^\top q = e_n^n$, and hence $q^\top = (q_1^\top \ q_2^\top) > 0$. And thus, apart from the origin, only e_n^n can form a nonobtuse simplex together with F_0 .

Remark 6.8 Note that this last argument does not hold if A_1 and A_2 are merely assumed to represent fully indecomposable nonobtuse simplices: the 9×9 matrix in Figure 15 shows that the normal of the facet opposite the origin may contain entries equal to zero.

To finish the case in which S has a matrix representation as in (44), assume without loss of generality that $A_1 = [1]$ and $A_2 \neq [1]$. Then the facet F of S opposite the last column of P lies in a cube facet, and thus it cannot have a nonobtuse face-to-face neighbor. For the remaining n facets of S , arguments as above apply, and we conclude that S has at most one nonobtuse neighbor at each of its facets. The remaining case that $A_1 = A_2 = [1]$ is trivial.

Note that if a nonobtuse 0/1-simplex has a block diagonal matrix representation with $p > 2$ blocks, each representing an acute simplex, the result remains valid, based on a similar proof.

Case II. Assume now that the matrix representation P of a nonobtuse 0/1-simplex S has the form

$$P = \begin{bmatrix} N_1 & 0 \\ 0 & A_1 \end{bmatrix}, \quad (45)$$

where $A_1 \in \mathbb{B}^{(n-k) \times (n-k)}$ represents an acute simplex and N_1 a merely nonobtuse simplex. Using similar arguments as in Case I it is easily seen that the only two choices of $v \in \mathbb{B}^n$ such

that $P^j(v)$ with $k+1 \leq j \leq n$ is nonobtuse are

$$v = Pe_j^n = \begin{bmatrix} 0 \\ a_j \end{bmatrix} \quad \text{and} \quad v = \begin{bmatrix} 0 \\ \frac{0}{a_j} \end{bmatrix}, \quad (46)$$

as no additional properties of N_1 need to be known. This changes if we examine the matrix $P^j(v)$ with $1 \leq j \leq k$, as it is generally not true that $N_1^\top N_1 > 0$. A way out is the following. Assume that also N_1 is partly decomposable, then using only row and column permutations, we can first transform N_1 into the form

$$N_1 \xrightarrow{(C)+(R)} \begin{bmatrix} N_2 & R \\ 0 & A_2 \end{bmatrix} \quad (47)$$

where we assume that A_2 represents an acute simplex. Then reflecting the vertex to the origin such that the block above A_2 becomes zero, we find that

$$P \sim \tilde{P} = \left[\begin{array}{c|c|c} N_2 & R & 0 \\ \hline 0 & A_2 & 0 \\ \hline 0 & 0 & A_1 \end{array} \right] \sim \left[\begin{array}{c|c|c} \tilde{N}_2 & 0 & \tilde{R} \\ \hline 0 & A_2 & 0 \\ \hline 0 & 0 & A_1 \end{array} \right] = \hat{P}, \quad (48)$$

where \tilde{R} has the same columns as R but possibly a different number of them. Now, select a column of \hat{P} that contains entries of A_2 and replace it by v , partitioned as $v^\top = (v_1^\top \ v_2^\top \ v_3^\top)$. Because the bottom right 2×2 block part of \hat{P} is a matrix representation of a nonobtuse simplex as considered in Case I, we conclude that $v_3 = 0$. Because the top left 2×2 block part of \hat{P} is a matrix representation as in (45), we conclude that $v_3 = 0$ and v_2 is a column of A_2 or its antipodal. Thus, also the facets of the vertices of S corresponding to its indecomposable part A_2 all have at most one nonobtuse neighbor.

Now, this process can be inductively repeated in case \tilde{N}_2 is partly decomposable with a fully indecomposable part that represents an acute simplex, and so on, until a fully indecomposable top left block A_p remains. This block presents vertices for which it still needs to be proved that their opposite facets have at most one nonobtuse neighbor. To illustrate how to do this, consider the case $p = 3$. Or, in other words, assume that N_2 in (48) represents an acute simplex. Replace one of the corresponding columns of \tilde{P} by v partitioned as $v^\top = (v_1^\top \ v_2^\top \ v_3^\top)$. Then $v_3 = 0$ because the $(1, 3)$ block of \tilde{P} equals zero. Similarly, because the $(1, 2)$ -block in \hat{P} equals zero, we find that $v_2 = 0$. And thus, v_3 is a column of N_2 or its antipodal. For $p > 3$, we can do the same one by one for the blocks at positions $(1, p), \dots, (1, 2)$.

The analysis in this section can be summarized in the following theorem.

Theorem 6.9 *Let S be a nonobtuse 0/1-simplex whose fully indecomposable components are all acute. Then S has at most one face-to-face neighbor at each of its interior facets.*

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